

Maximum atom-bond connectivity index with given graph parameters *

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Abstract

The atom-bond connectivity (ABC) index is a degree-based topological index. It was introduced due to its applications in modeling the properties of certain molecular structures and has been since extensively studied. In this note, we examine the influence on the extremal values of the ABC index by various graph parameters. More specifically, we consider the maximum ABC index of connected graphs of given order, with fixed independence number, number of pendent vertices, chromatic number and edge-connectivity respectively. We provide characterizations of extremal structures as well as some conjectures. Numerical analysis of the extremal values are also presented.

Key words: Atom-bond connectivity index; independence number; pendent vertices; chromatic number; edge-connectivity

AMS Classifications: 05C05, 05C30

1 Introduction and preliminaries

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, the degree of u , denoted by $d(u)$, is the number of neighbors of u in

*This work is supported by the National Natural Science Foundation of China (Nos.11531001 and 11271256), the Joint NSFC-ISF Research Program (jointly funded by the National Natural Science Foundation of China and the Israel Science Foundation(No. 11561141001)), Innovation Program of Shanghai Municipal Education Commission (No. 14ZZ016, No. 15ZZ108), and Simons Foundation (No. 245307).

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G . An independent set is a set of vertices of which no pair is adjacent. The independence number $\beta(G)$ of a graph G is the size of a largest independent set of G . The chromatic number $\chi(G)$ of a graph G is the least number of colors assigned to $V(G)$ such that no adjacent elements receive the same color. The edge connectivity $k(G)$ of a graph G is the minimum number of edges needed to disconnect G .

The atom bond connectivity (ABC) index of G is defined [8] as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}.$$

The ABC index is one of many so called topological indices that are extensively used in theoretical chemistry to correlate physico-chemical properties with the molecular structures of chemical compounds. It appears that the ABC index shows a strong correlation with heat of formation of alkanes [8]. Some topological approaches were also developed basing on the ABC index to explain the differences in the energy of linear and branched alkanes [7].

In the study of topological indices in general, it is often of interest to consider the extremal values of a certain index among graphs under various constrains. Along this line, the extremal values of the ABC index have been extensively explored [2–6, 9–16].

We intend to expand this study by exploring the maximum ABC index of connected graphs of given order, with fixed independence number, number of pendent vertices, edge-connectivity, and chromatic number respectively. First we will introduce some simple but useful facts.

Theorem 1.1 ([1]). *Let G be a graph with n vertices, if $x, y \in V(G)$ and $xy \in E(\overline{G})$, then*

$$ABC(G) \leqslant ABC(G + xy)$$

with equality if and only if x and y are both isolated vertices. Furthermore,

$$ABC(G) \leqslant ABC(K_n)$$

with equality if and only if $G = K_n$.

To simplify notations, we define the following functions:

- $f(x, y) = \sqrt{\frac{x+y-2}{xy}};$
- $g(x, y) = f(x+1, y) - f(x, y);$
- $F(x) = xf(x+m, 1),$

for $x, y, m \geq 1$.

Lemma 1.2 ([14]). *For the function $f(x, y)$ we have:*

- $f(x, 1)$ is strictly increasing with respect to x ;

- $f(x, 2) = \frac{\sqrt{2}}{2}$;
- $f(x, y)$ is strictly decreasing with respect to x for any fixed $y \geq 3$.

Lemma 1.3 ([4, 14]). *The function $g(x, y)$ is strictly decreasing with respect to x if $y = 1$, and increasing with respect to x if $y \geq 2$.*

Lemma 1.4. *The function $F(x)$ is convex and strictly increasing for $x \geq 1$. As a result of the convexity we have*

$$F(x_1 + 1) - F(x_1) > F(x_2) - F(x_2 - 1)$$

if $x_1 \geq x_2 \geq 1$.

Proof. Note that $F(x) = xf(x + m, 1) = x\sqrt{\frac{x+m-1}{x+m}}$, then we have

$$\begin{aligned} F'(x) &= \sqrt{\frac{x+m-1}{x+m}} + \frac{x}{2} \cdot \sqrt{\frac{x+m}{x+m-1}} \cdot \frac{1}{(x+m)^2} \\ &= \sqrt{\frac{x+m-1}{x+m}} \left(1 + \frac{1}{2} \cdot \frac{x}{(x+m-1)(x+m)} \right) > 0 \end{aligned}$$

and

$$\begin{aligned} F''(x) &= \frac{1}{2} \cdot \sqrt{\frac{x+m}{x+m-1}} \cdot \frac{1}{(x+m)^2} \left(1 + \frac{1}{2} \left(\frac{m}{x+m} - \frac{m-1}{x+m-1} \right) \right) \\ &\quad + \sqrt{\frac{x+m-1}{x+m}} \left(-\frac{m}{2(x+m)^2} + \frac{m-1}{2(x+m-1)^2} \right) \\ &= \sqrt{\frac{x+m-1}{x+m}} \left(\frac{1 + \frac{1}{2}(\frac{m}{x+m} - \frac{m-1}{x+m-1})}{2(x+m-1)(x+m)} - \frac{m}{2(x+m)^2} + \frac{m-1}{2(x+m-1)^2} \right) \\ &= \frac{(4m-1)x + 4m(m-1)}{4(x+m)^{\frac{5}{2}}(x+m-1)^{\frac{3}{2}}} > 0 \end{aligned}$$

when $x, m \geq 1$. □

Lemma 1.5. *Let $G(a, b) = f(a, b-1) - f(a-1, b)$ for some $a > b > 0$. Then $G(a, b) > 0$.*

Proof. This follows from direct calculations. □

In the following sections we will first explore the maximum ABC index of graphs of given order and various fixed parameters. Based on these results some computational analysis is provided. In the end we briefly discuss some other questions and pose a couple of conjectures.

2 Maximum ABC index with given independence number or number of pendent vertices

In this section we characterize the extremal graph on n vertices, with given independence number (Theorem 2.2) and with given number of pendent vertices (Theorem 2.4).

Definition 2.1. For two vertex-disjoint graphs G and H , the join of G and H , denoted by $G \vee H$, is a graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H) \cup \{xy \mid x \in V(G), y \in V(H)\}$.

Theorem 2.2. Let G be a connected graph on n vertices and independence number β . Then

$$ABC(G) \leq \beta(n - \beta) \sqrt{\frac{2n - \beta - 3}{(n - \beta)(n - 1)}} + \frac{(n - \beta)(n - \beta - 1)}{2} \sqrt{\frac{2n - 4}{(n - 1)(n - 1)}}$$

with equality if and only if $G \cong \overline{K_\beta} \vee K_{n-\beta}$.

Proof. Suppose G^* is the graph with the maximum ABC index among all n -vertex connected graphs with independence number β .

Let S be a maximal independent set in G^* with $|S| = \beta$. By Theorem 1.1, adding edges to a graph will increase its ABC index. Thus each vertex x in S is adjacent to every vertex y in $G^* - S$ and the subgraph induced by vertices in $G^* - S$ is $K_{n-\beta}$. Consequently $G^* \cong \overline{K_\beta} \vee K_{n-\beta}$. Direct calculations yield

$$\begin{aligned} & ABC(\overline{K_\beta} \vee K_{n-\beta}) \\ &= \beta(n - \beta) \sqrt{\frac{2n - \beta - 3}{(n - \beta)(n - 1)}} + \frac{(n - \beta)(n - \beta - 1)}{2} \sqrt{\frac{2n - 4}{(n - 1)(n - 1)}}. \end{aligned}$$

□

Definition 2.3. For convenience we employ the following notations:

- let K_n^p denote the graph obtained from attaching p pendent edges to one vertex of K_{n-p} ; and
- let G' denote the graph obtained from attaching $n - 3$ pendent edges to one end of a path on three vertices.

Theorem 2.4. Let G be a connected graph on n vertices with p pendent vertices, then:

1. If $n - p = 1$, then $ABC(G) = ABC(S_n) = \sqrt{(n - 1)(n - 2)}$;
2. If $n - p = 2$, then $ABC(G) \leq (n - 3) \sqrt{\frac{n - 3}{n - 2}} + \sqrt{2}$ with equality if and only if $G \cong G'$;

3. If $n - p > 2$, then

$$ABC(G) \leq p\sqrt{\frac{n-2}{n-1}} + (n-p-1)\sqrt{\frac{2n-p-4}{(n-1)(n-p-1)}} \\ + \frac{(n-p-1)(n-p-2)}{2}\sqrt{\frac{2n-2p-4}{(n-p-1)^2}}$$

with equality if and only if $G \cong K_n^p$.

Proof. Let G^* be the graph with the maximum ABC index among all n -vertex connected graphs with p pendent vertices.

Case 1: If $n - p = 1$, then G^* is the star.

Case 2: If $n - p = 2$, then G^* is the graph obtained by attaching a_1 pendent edges to one vertex v_1 and $a_2 (= p - a_1)$ pendent edges to the other vertex v_2 of K_2 .

Assuming, without loss of generality, that $a_1 \geq a_2 \geq 1$, we claim that $a_1 = p - 1 = n - 3$ and $a_2 = 1$ (note that in this case $G^* \cong G'$).

Otherwise, if $a_2 \geq 2$, let G_1 be obtained from G^* by detaching and reattaching one of the pendent edges from v_2 to v_1 . Then

$$ABC(G_1) - ABC(G^*) = ((a_1 + 1)f((a_1 + 1) + 1, 1) - a_1 f(a_1 + 1, 1)) \\ - (a_2 f(a_2 + 1, 1) - (a_2 - 1)f((a_2 - 1) + 1, 1)) \\ + (f(a_1 + 2, a_2) - f(a_1 + 1, a_2 + 1)).$$

Let $x_1 = a_1$, $x_2 = a_2$ and $m = 1$ in Lemma 1.4, we have

$$F(a_1 + 1, 1) - F(a_1, 1) > F(a_2, 1) - F(a_2 - 1, 1).$$

Or equivalently,

$$(a_1 + 1)f((a_1 + 1) + 1, 1) - a_1 f(a_1 + 1, 1) \\ - (a_2 f(a_2 + 1, 1) - (a_2 - 1)f((a_2 - 1) + 1, 1)) > 0.$$

Applying Lemma 1.5 with $a = a_1 + 2$ and $b = a_2 + 1$ yields $f(a_1 + 2, a_2) - f(a_1 + 1, a_2 + 1) > 0$.

Consequently $ABC(G_1) - ABC(G^*) > 0$, a contradiction. The conclusion then follows from direct calculations.

Case 3: If $n - p > 2$, let P be the set of pendent vertices in G^* with $|P| = p$. Again by Theorem 1.1, the subgraph induced by vertices in $G^* - P$ must be K_{n-p} . Label the vertices of this K_{n-p} as v_1, v_2, \dots, v_{n-p} and let the number of pendent vertices adjacent to each vertex v_i be a_i with $a_1 \geq a_2 \geq \dots \geq a_{n-p} \geq 0$.

If $a_1 = p$ and $a_2 = \dots = a_{n-p} = 0$, then $G^* \cong K_n^p$.

If $G^* \not\cong K_n^p$, then $a_1 \geq a_2 \geq 1$. Consider G_2 obtained from detaching one of

the pendent edges of v_2 and reattaching to v_1 . We have

$$\begin{aligned}
& ABC(G_2) - ABC(G^*) \\
&= \sum_{i=3}^{n-p} [(f(a_1 + n - p, a_i + n - p - 1) - f(a_1 + n - p - 1, a_i + n - p - 1)) \\
&\quad - (f(a_2 + n - p - 1, a_i + n - p - 1) - f(a_2 + n - p - 2, a_i + n - p - 1))] \\
&\quad + (f(a_1 + n - p, a_2 + n - p - 2) - f(a_1 + n - p - 1, a_2 + n - p - 1)) \\
&\quad + ((a_1 + 1)f((a_1 + 1) + n - p - 1, 1) - a_1 f(a_1 + n - p - 1, 1)) \\
&\quad - (a_2 f(a_2 + n - p - 1, 1) - (a_2 - 1)f((a_2 - 1) + n - p - 1, 1)).
\end{aligned}$$

For each $i = 3, 4, \dots, n - p$, we have $a_i + n - p - 1 \geq 2$, $a_1 + n - p - 2 \geq 2$ and $a_1 + n - p - 1 > a_2 + n - p - 2$. Then by Lemma 1.3,

$$\begin{aligned}
& (f(a_1 + n - p, a_i + n - p - 1) - f(a_1 + n - p - 1, a_i + n - p - 1)) \\
&\quad - (f(a_2 + n - p - 1, a_i + n - p - 1) - f(a_2 + n - p - 2, a_i + n - p - 1)) \\
&\quad \geq 0.
\end{aligned}$$

From $a_1 + n - p > a_2 + n - p - 1$ and Lemma 1.5, we have

$$\begin{aligned}
& G(a_1 + n - p, a_2 + n - p - 1) \\
&= f(a_1 + n - p, a_2 + n - p - 2) - f(a_1 + n - p - 1, a_2 + n - p - 1) > 0.
\end{aligned}$$

Let $m = n - p - 1$, by Lemma 1.4, we have

$$F(a_1 + 1) - F(a_1) > F(a_2) - F(a_2 - 1)$$

for $a_1 \geq a_2$.

As a consequence we have

$$\begin{aligned}
& ((a_1 + 1)f((a_1 + 1) + n - p - 1, 1) - a_1 f(a_1 + n - p - 1, 1)) \\
&\quad - (a_2 f(a_2 + n - p - 1, 1) - (a_2 - 1)f((a_2 - 1) + n - p - 1, 1)) > 0
\end{aligned}$$

and hence $ABC(G_2) - ABC(G^*) > 0$, a contradiction. Thus $G \cong K_n^p$ and the conclusion follows. \square

3 Maximum ABC index with given edge-connectivity

In this section we consider the maximum ABC index of graphs of given order and edge-connectivity. The conclusion is, to some extent, expected. But the proof turned out to be rather complicated.

Theorem 3.1. *Let G be a connected graph on $n \geq 6$ vertices and edge-connectivity $k \geq 2$. Then*

$$ABC(G) \leq k \sqrt{\frac{n+k-3}{k(n-1)}} + \frac{k(k-1)}{2(n-1)} \sqrt{2n-4} + \frac{(n-k-1)(n-k-2)}{2(n-2)} \sqrt{2n-6}$$

$$+k(n-k-1)\sqrt{\frac{2n-5}{(n-1)(n-2)}}$$

with equality if and only if $G \cong K_k \vee (K_1 + K_{n-k-1})$.

Note that $K_k \vee (K_1 + K_{n-k-1})$ is simply the graph obtained from joining one vertex with k of the vertices in K_{n-1} .

Proof. Suppose G^* is the graph with maximum ABC index among all graphs of order $n \geq 6$ and edge-connectivity $k \geq 2$, let e_1, e_2, \dots, e_k be a k -edge cut in G^* and let G_1, G_2 be the connected components in $G^* - \{e_1, e_2, \dots, e_k\}$. Again by Theorem 1.1, both G_1 and G_2 must be complete graphs. Let n_i be the number of vertices of G_i ($i = 1, 2$), then $n_1 + n_2 = n$.

Without loss of generality, let $n_2 \geq n_1$. If $n_1 = 1$, then $G^* \cong K_k \vee (K_1 + K_{n-k-1})$.

Now we focus on the case of $n_2 \geq n_1 \geq 2$. For $i = 1, 2$, G_i has $\frac{n_i(n_i-1)}{2}$ edges, for G_i is a complete graph. On the other hand, the sum of degrees of all vertices in G_i is at least $n_i k$, for the minimum degree of G^* is at least k . Thus G_i has at least $\frac{n_i k - k}{2}$ edges. Hence $\frac{n_i(n_i-1)}{2} \geq \frac{n_i k - k}{2} = \frac{k(n_i-1)}{2}$, implying that $n_i \geq k$. Consequently we can assume $n_2 \geq n_1 \geq k$.

Firstly, if there is a vertex, say v in $V(G^*)$, of degree k . Let v_1, \dots, v_k be the neighbors of v . Write $A = \{v_1, \dots, v_k\}$ and $B = V(G^*) \setminus \{v, v_1, \dots, v_k\}$. If $G[A \cup B]$, the subgraph of G^* induced by $V(A \cup B)$, is the complete graph K_{n-1} , then $G^* \cong K_k \vee (K_1 + K_{n-k-1})$ as claimed.

Otherwise, there exist $x, y \in V(G^*)$ such $xy \in E(\overline{G[A \cup B]})$. But then the graph $G' = G^* + xy$ still have edge-connectivity k with $ABC(G') > ABC(G^*)$ by Theorem 1.1, contradiction.

If, on the other hand, $d_{G^*}(v) \geq k+1$ for every vertex $v \in V(G^*)$. Then we must have $n_2 \geq n_1 \geq k+1$ by similar arguments. We now show that the maximum ABC index cannot be achieved in this case.

If $n_2 \geq n_1 \geq k+1 \geq 3$, by Lemma 1.2 we have

$$\begin{aligned} ABC(G^*) &< \frac{n_1(n_1-1)}{2} f(n_1-1, n_1-1) \\ &\quad + \frac{n_2(n_2-1)}{2} f(n_2-1, n_2-1) + k f(n_1, n_2) \\ &< \frac{n_1^{\frac{3}{2}}}{\sqrt{2}} + \frac{n_2^{\frac{3}{2}}}{\sqrt{2}} + k \sqrt{\frac{n_1+n_2-2}{n_1 n_2}}. \end{aligned}$$

Note that when $n_1 = 1$, also by Lemma 1.2 we have

$$\begin{aligned}
ABC(G^*) &> kf(k, n-1) + \frac{(n-1)(n-2)}{2} f(n-1, n-1) \\
&= k\sqrt{\frac{n+k-3}{k(n-1)}} + \frac{(n-1)(n-2)}{2} \sqrt{\frac{2(n-2)}{(n-1)(n-1)}} \\
&= k\sqrt{\frac{n+k-3}{k(n-1)}} + \frac{(n-2)^{\frac{3}{2}}}{\sqrt{2}}.
\end{aligned}$$

We now make use of the following fact.

Claim 3.2. For $n \geq 10$ and $3 \leq k+1 \leq n_1 \leq \frac{n}{2}$,

$$k\sqrt{\frac{n+k-3}{k(n-1)}} + \frac{(n-2)^{\frac{3}{2}}}{\sqrt{2}} > \frac{n_1^{\frac{3}{2}}}{\sqrt{2}} + \frac{n_2^{\frac{3}{2}}}{\sqrt{2}} + k\sqrt{\frac{n_1+n_2-2}{n_1n_2}}. \quad (1)$$

Note that our conclusion follows from (1). For $6 \leq n \leq 9$, it is easy to check that the case $n_1 = 1$ yields larger ABC index than the case $n_1 \geq k+1$, for each $2 \leq k \leq \frac{n}{2} - 1$. \square

In the rest of this section we provide a proof to (1).

Proof of Claim 3.2. First note that (1) is equivalent to

$$(n-2)^{\frac{3}{2}} - (n_1^{\frac{3}{2}} + (n-n_1)^{\frac{3}{2}}) > \sqrt{2}k \left(\sqrt{\frac{n-2}{n_1(n-n_1)}} - \sqrt{\frac{n+k-3}{k(n-1)}} \right).$$

For $3 \leq k+1 \leq n_1 \leq \frac{n}{2}$, let

$$h(n, n_1) = (n-2)^{\frac{3}{2}} - (n_1^{\frac{3}{2}} + (n-n_1)^{\frac{3}{2}})$$

and

$$l(n, k, n_1) = \sqrt{2}k \left(\sqrt{\frac{n-2}{n_1(n-n_1)}} - \sqrt{\frac{n+k-3}{k(n-1)}} \right).$$

Then $h(n, n_1)$ is strictly increasing and $l(n, k, n_1)$ is strictly decreasing for $3 \leq k+1 \leq n_1 \leq \frac{n}{2}$. Hence

$$h(n, n_1) \geq h(n, k+1) \geq h(n, 3) = (n-2)^{\frac{3}{2}} - (3^{\frac{3}{2}} + (n-3)^{\frac{3}{2}})$$

and $l(n, k, n_1) \leq l(n, k, k+1)$.

We now show that

$$l(n, k, k+1) = \sqrt{2}k \left(\sqrt{\frac{n-2}{(k+1)(n-k-1)}} - \sqrt{\frac{n+k-3}{k(n-1)}} \right)$$

is increasing for $2 \leq k \leq \frac{n}{2} - 1$ and $n \geq 20$.

It is easy to obtain the formula (which we skip for it is too long and not informative) of $l'_k(n, k, k+1)$, and see (with the help of computer) that $l'_k(n, k, k+1)$ is positive for some particular values of k and n . We may claim that $l'_k(n, k, k+1)$ is positive for $2 \leq k \leq \frac{n}{2} - 1$ and $n \geq 20$ by showing $l'_k(n, k, k+1) = 0$ is not possible (and hence $l'_k(n, k, k+1)$ must be always positive).

Thanks to computer algebra, we have that $l'_k(n, k, k+1) = 0$ is equivalent to

$$\begin{aligned} 0 = & (k^2 + k - 1)n^5 - (8k^2 + 6k - 9)n^4 + (5k^5 + 8k^4 + 19k^2 + 6k - 30)n^3 \\ & + (k^6 - 24k^5 - 42k^4 - 2k^3 - 3k^2 + 20k + 46)n^2 \\ & - (8k^7 + 6k^6 - 57k^5 - 75k^4 + 10k^3 + 36k^2 + 39k + 33)n \\ & + 4k^8 + 12k^7 - 3k^6 - 46k^5 - 37k^4 + 16k^3 + 27k^2 + 18k + 9, \end{aligned}$$

or equivalently

$$\begin{aligned} 0 = & ((k^2 + k - 1)n^5 - (8k^2 + 6k - 9)n^4) \\ & + [(k^5 + 8k^4 + 19k^2 + 6k - 30)n^3 \\ & \quad - (24k^5 + 42k^4 + 2k^3 + 3k^2 - 20k - 46)n^2] \\ & + [(57k^5 + 75k^4 - 10k^3 - 36k^2 - 39k - 33)n \\ & \quad - (46k^5 + 37k^4 - 16k^3 - 27k^2 - 18k - 9)] \\ & + (4k^5n^3 + k^6n^2 - (8k^7 + 6k^6)n) + 4k^8 + 12k^7 - 3k^6. \end{aligned}$$

For simplicity we denote the above expression by $H(n, k)$. It is then straightforward to check the followings:

- $(k^2 + k - 1)n^5 - (8k^2 + 6k - 9)n^4 > 0$ when $n \geq 8$;
- $(k^5 + 8k^4 + 19k^2 + 6k - 30)n^3 - (24k^5 + 42k^4 + 2k^3 + 3k^2 - 20k - 46)n^2 > 0$ when $n \geq 24$;
- for $2 \leq k < \frac{n}{2}$, we have $4k^8 + 12k^7 - 3k^6 > 0$ and $4k^5n^3 + k^6n^2 - (8k^7 + 6k^6)n > 0$;
- for $20 \leq n \leq 23$, simple calculation shows $H(n, k) > 0$.

Thus, $l(n, k, k+1)$ is increasing when $n \geq 20$ and $2 \leq k \leq \frac{n}{2} - 1$.

Consequently

$$l(n, k, k+1) \leq l(n, \frac{n}{2} - 1, \frac{n}{2})$$

when n is even and

$$l(n, k, n_1) \leq l(n, k, k+1) \leq l(n, \frac{n-1}{2} - 1, \frac{n-1}{2})$$

when n is odd. We now discuss different cases to finish the proof:

- If $10 \leq n \leq 13$, the case $n_1 = 1$ yields larger ABC index than the case $n_1 \geq k+1 = 3$ and we always have $h(n, k+1) \geq l(n, k, k+1)$ for $3 \leq k \leq \frac{n}{2} - 1$;
- If $14 \leq n \leq 19$, we always have $h(n, k+1) \geq l(n, k, k+1)$ for $2 \leq k \leq \frac{n}{2} - 1$;
- If $20 \leq n \leq 48$, we always have $h(n, 3) \geq l(n, \frac{n}{2} - 1, \frac{n}{2})$ when n is even and $h(n, 3) \geq l(n, \frac{n-1}{2} - 1, \frac{n-1}{2})$ when n is odd;
- If $n \geq 49$, we have

$$\begin{aligned}
h(n, 3) &= (n-2)^{\frac{3}{2}} - (3^{\frac{3}{2}} + (n-3)^{\frac{3}{2}}) \\
&= \frac{3n^2 - 15n + 19}{\sqrt{n^3 - 6n^2 + 12n - 8} + \sqrt{n^3 - 9n^2 + 27n - 27}} - 3^{\frac{3}{2}} \\
&> \frac{3n^2 - 15n + 19}{\sqrt{n^3} + \sqrt{n^3}} - 3^{\frac{3}{2}} \\
&> \frac{3}{2}(n^{\frac{1}{2}} - 5n^{-\frac{1}{2}}) - 3^{\frac{3}{2}}.
\end{aligned}$$

On the other hand,

$$\begin{aligned}
&l\left(n, \frac{n}{2} - 1, \frac{n}{2}\right) \\
&= \sqrt{2}\left(\frac{n}{2} - 1\right) \left(\sqrt{\frac{n-2}{\frac{n}{2}(n-\frac{n}{2})}} - \sqrt{\frac{n+\frac{n}{2}-1-3}{(\frac{n}{2}-1)(n-1)}} \right) \\
&< \frac{\sqrt{2n}}{2} \frac{n^3 - 12n^2 + 32n - 16}{2\sqrt{n^6 - 6n^5 + 13n^4 - 12n^3 + 4n^2} + \sqrt{3n^6 - 11n^5 + 8n^4}} \\
&< \frac{\sqrt{2n}}{2} \frac{1 + 32n^{-2}}{2\sqrt{1 - 6n^{-1}} + \sqrt{3 - 11n^{-1}}} \\
&\leq \frac{\sqrt{2n}}{2} \frac{1 + 32n^{-2}}{2\sqrt{1 - 6 \times 49^{-1}} + \sqrt{3 - 11 \times 49^{-1}}} \\
&= \frac{\sqrt{2n}}{2} \frac{7}{2\sqrt{43} + \sqrt{136}} (1 + 32n^{-2}) \\
&< 0.2n^{\frac{1}{2}} + 7n^{-\frac{3}{2}}
\end{aligned}$$

when n is even. For $n \geq 49$, it is easy to see that

$$1.3n^{\frac{1}{2}} > 7.5n^{-\frac{1}{2}} + 3^{\frac{3}{2}} + 7n^{-\frac{3}{2}}$$

and hence

$$\frac{3}{2} \left(n^{\frac{1}{2}} - 5n^{-\frac{1}{2}} \right) - 3^{\frac{3}{2}} > 0.2n^{\frac{1}{2}} + 7n^{-\frac{3}{2}}.$$

Similarly, when n is odd,

$$\begin{aligned}
& l\left(n, \frac{n-1}{2} - 1, \frac{n}{2}\right) \\
&= \sqrt{2} \left(\frac{n-1}{2} - 1\right) \left(\sqrt{\frac{n-2}{\frac{n-1}{2}(n - \frac{n-1}{2})}} - \sqrt{\frac{\frac{3n-9}{2}}{\frac{(n-3)}{2}(n-1)}} \right) \\
&= \frac{\sqrt{2}}{2} (n-3) \frac{\frac{4(n-2)}{n^2-1} - \frac{3}{n-1}}{\sqrt{\frac{4(n-2)}{n^2-1}} + \sqrt{\frac{3}{n-1}}} \\
&= \frac{\sqrt{2}}{2} \frac{n^2 - 14n + 33}{\sqrt{4(n^3 - 2n^2 - n + 2)} + \sqrt{3(n^3 + n^2 - n - 1)}}.
\end{aligned}$$

Then

$$\begin{aligned}
& l\left(n, \frac{n-1}{2} - 1, \frac{n}{2}\right) \\
&< \frac{\sqrt{2}}{2} \frac{n^2 + 33}{\sqrt{4(n^3 - 3n^2)} + \sqrt{3n^3}} \\
&= \frac{\sqrt{2}}{2} \frac{n^{\frac{1}{2}} + 33n^{-\frac{3}{2}}}{\sqrt{4(1 - 3n^{-1})} + \sqrt{3}} \\
&\leq \frac{\sqrt{2}}{2} \frac{1}{\sqrt{4(1 - \frac{3}{49})} + \sqrt{3}} \left(n^{\frac{1}{2}} + 33n^{-\frac{3}{2}}\right) \\
&= \frac{\sqrt{2}}{2} \frac{7}{2\sqrt{46} + 7\sqrt{3}} \left(n^{\frac{1}{2}} + 33n^{-\frac{3}{2}}\right) \\
&< 0.2 \left(n^{\frac{1}{2}} + 33n^{-\frac{3}{2}}\right).
\end{aligned}$$

For $n \geq 49$ we have

$$1.3n^{\frac{1}{2}} > 7.5n^{-\frac{1}{2}} + 3^{\frac{3}{2}} + 6.6n^{-\frac{3}{2}}$$

and hence

$$\frac{3}{2} \left(n^{\frac{1}{2}} - 5n^{-\frac{1}{2}}\right) - 3^{\frac{3}{2}} > 0.2 \left(n^{\frac{1}{2}} + 33n^{-\frac{3}{2}}\right).$$

□

4 Some computational analysis

With Theorems 2.2, 2.4 and 3.1, we may examine the influence on the maximum ABC index by the independence number β , pendent vertex number p , and edge-connectivity number k . In Figure 1 we take $n = 200, 250, 300, 350$ respectively

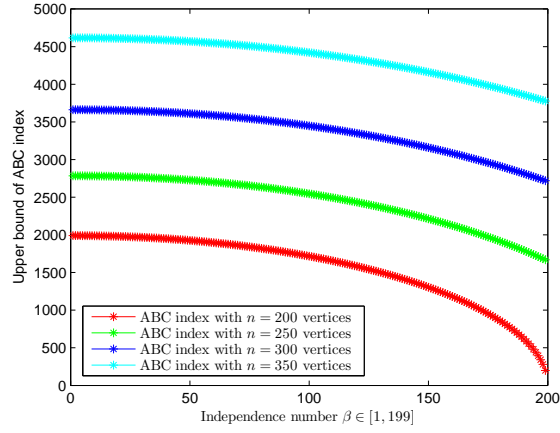


Figure 1: The maximum ABC index with $n = 200, 250, 300, 350$ and $\beta \in [1, 199]$.

and $\beta \in [1, 199]$, it is easy to see that the maximum ABC index is decreasing faster as β grows.

Similarly, Figures 2 and 3 show that the maximum ABC index decreases, but slower as the number of pendant vertices or edge-connectivity grows.

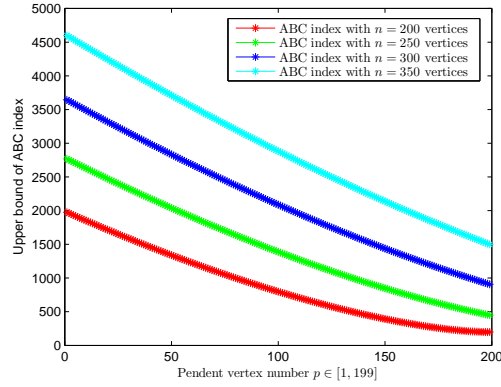


Figure 2: The maximum ABC index with $n = 200, 250, 300, 350$ and $p \in [1, 199]$.

In Figure 4 the curves corresponding to $n = 200$, $\beta, p \in [1, 199]$, and $k \in [2, 199]$ are plotted. It is interesting to note that with given value x , the maximum ABC index is the largest when $\beta = x$ and smallest when $k = x$.

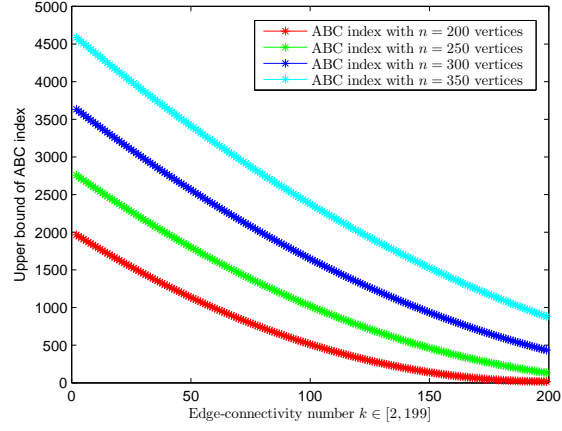


Figure 3: The maximum ABC index with $n = 200, 250, 300, 350$ and $k \in [2, 199]$.

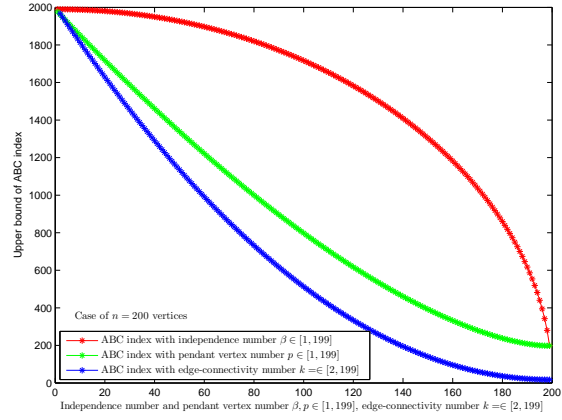


Figure 4: The maximum ABC index with $n = 200$, $\beta, p \in [1, 199]$, and $k \in [2, 199]$.

5 Concluding Remarks

We have discussed the maximum ABC index among graphs of given order and various fixed parameters. As can be seen from the arguments, the ideas are simple but the proofs can be very technical and tedious. As another example of such studies, one may consider the maximum ABC index of graphs with given chromatic number.

Definition 5.1. Denote by $T_{n,t}$ the complete t -partite graph of order n with $|n_i - n_j| \leq 1$, where n_i , $i = 1, 2, \dots, t$, is the number of vertices in the i th partition set of $T_{n,t}$.

Proposition 5.2. For any connected graph G of order n with chromatic number $\chi = 2$:

- If n is even, then $ABC(G) \leq \frac{n}{2}\sqrt{n-2}$ with equality if and only if $G \cong T_{n,2}$;
- If n is odd, then $ABC(G) \leq \frac{1}{2}\sqrt{(n-2)(n^2-1)}$ with equality if and only if $G \cong T_{n,2}$.

Proof. Let G^* be the graph with the maximum ABC index among all n -vertex connected graphs with chromatic number $\chi = 2$. By Theorem 1.1, we must have $G^* \cong \overline{K_{n_1}} \vee \overline{K_{n_2}}$, where n_i is the number of vertices in the i th partition set.

Suppose (for contradiction) that $G^* \not\cong T_{n,2}$ and $n_2 \geq n_1 + 2$, consider $G' = \overline{K_{n_1+1}} \vee \overline{K_{n_2-1}}$ and we have

$$\begin{aligned} & ABC(G') - ABC(G^*) \\ &= (n_1 + 1)(n_2 - 1) \sqrt{\frac{2n - n_1 - n_2 - 2}{(n_1 + 1)(n_2 - 1)}} - n_1 n_2 \sqrt{\frac{2n - n_1 - n_2 - 2}{n_1 n_2}} \\ &= \left(\sqrt{(n_1 + 1)(n_2 - 1)} - \sqrt{n_1 n_2} \right) \sqrt{n - 2}. \end{aligned}$$

Since $(n_1 + 1)(n_2 - 1) - n_1 n_2 = n_2 - n_1 - 1 > 0$, we have $ABC(G') - ABC(G^*) > 0$, a contradiction. \square

Both computational results and combinatorial intuitions suggest the following, which we post here as a conjecture.

Conjecture 5.3. Let G be an n -vertex connected graph with chromatic number $\chi \geq 3$. Then

$$ABC(G) \leq ABC(T_{n,\chi})$$

with equality if and only if $ABC(G) \cong ABC(T_{n,\chi})$.

Another question is to consider the case when the edge connectivity is 1. We conjecture that the maximum ABC index behaves similarly as in the general case, achieved by attaching a pendant edge to a vertex of K_{n-1} . Note that

to prove this, it suffices to show that the following function (with $f(x, y) = \sqrt{\frac{x+y-2}{xy}}$) is decreasing:

$$\begin{aligned} & (x-1)f(x, x-1) + \frac{1}{2}(x-1)(x-2)f(x-1, x-1) + f(x, n-x) \\ & + (n-x-1)f(n-x, n-x-1) \\ & + \frac{1}{2}(n-x-1)(n-x-2)f(n-x-1, n-x-1). \end{aligned}$$

Acknowledgements

The authors would like to thank the anonymous referees for many helpful and comments on an earlier version of this paper.

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